Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0202010

FWP and possible subtask under FWP:
Complex deformation in metals; modeling and measurement

FWP Number: 04SCPE424

Program Scope: The goal of this project is the validated prediction of macroscale mechanical response of polycrystalline metals. Using SMARTS and HIPPO, two state of the art neutron diffractometers at Los Alamos, we measure microstructural deformation and texture evolution. The results test assumptions (pursuant to slip, twinning, creep, grain refinement and grain rotation) used in elastoplastic and viscoplastic self consistent models, the combination of which determine macroscopic material properties. Current focus areas include; equichannel angular processed Al & Ni & Be, texture development and constitutive performance of low symmetry materials that can deform by twinning (NiTi, Mg, U6Nb & Zr), load sharing in bulk metallic glass composites (Vitreloy-W) and creep of Ni base superaloys.

Major Program Achievements (over duration of support):
The scope of this project encompasses many different polycrystalline systems which include but are not limited to;

- In situ deformation studies on composites such as Ti-SiC, Al-TiC NiAl-AlN-Al2O3, NiTi-TiC, Cu-Mo, WC-Co and γ–γ' Ni base superalloys have provided insights about co-deformation behavior and quantified the effects of residual stress on macroscopic performance.
- Studies on "shape memory" super-elastic and thermo-elastic NiTi and NiTiTiC have shown for the first time the texture evolution of the stress induced phase.
- Model descriptions of twinning have been added to the visco-plastic self consistent models and shown to predict the constitutive performance of cross rolled zirconium deformed under a variety of temperature and strain rate conditions. The phenomenology is being extended to other systems including Mg and U6Nb.

Program Impact:

- Construction of the SMARTS diffractometer at the Lujan center which is a direct result of the success of this FWP. SMARTS is used by approximately 30 external users per year to make unique measurements on a wide cross section of engineering materials
- PI is a Met Trans key reader, member of the Vulcan IDT (comparable instrument to SMARTS scheduled for SNS), Co-organizer of TMS 03 symposium, & Meca Sens international organizing committee
- Award of LANL LDRD to study ECAP
- Focus for US neutron scattering studies on engineering materials

Interactions:
California Institute of Technology (Prof. Ersan Ustundag)
Northwestern University (Prof David. Dunand)
University of central Florida (Prof. Raj Vaidyanathan)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2002 DP Award of Excellence, Beryllium Stress Measurements
Best graduate paper at the MRS Annual RioGrande Conference in Albuquerque (October 2002)
First place, 2000 MST Division Review Poster Session,
Jerome B. Cohen Student Award For Best Paper at the Denver X-ray Conference 2000
17th Annual Louis Rosen Award for outstanding doctoral thesis (1999)
2nd place in GKSS Research Center Prize "Verständliche Wissenschaft" ("Understandable Science")

Personnel Commitments for FY2002 to Nearest +/-10%:
Mark Bourke (Team leader) 50%, Don Brown (TSM) 40%, Sven Vogel (Postdoc) 100%, Bjorn Clausen (Postdoc) 50%, Thomas Sisneros (Tec) 30%, Thomas Holden (Mathias Scholar) 60% but independent funding

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $554,000 **FY01 BA** $608,0000 **FY02 BA** $580,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0202010

FWP and possible subtask under FWP:
Complex Electronic Materials

FWP Number: O4SCPE355

Program Scope: Research focuses on developing a fundamental understanding of the physics of complex and collective states in electronic materials by discovering new materials that reveal essential new physics. A necessarily broad range of experimental techniques, especially neutron scattering and often at extremes of low temperatures, high fields and high pressures, is used to probe static and dynamic spin, charge and lattice degrees-of-freedom and their interactions on multiple length and time scales. Particular attention is given to highly correlated f-electron materials and high temperature superconductors, often in single crystal form, as exemplary complex electronic materials.

Major Program Achievements (over duration of support): Established the study of heavy-fermion materials as a new field of condensed matter physics through discoveries of numerous examples of unconventional superconducting, magnetic and semiconducting states in new correlated f-electron systems, culminating in the recent discovery of superconductivity in $PuCoGa_5$; discovered high T_c superconductivity in rare-earth cuprates, providing the first indication for the importance of CuO_2 planes; pioneered the now widely accepted importance of intrinsic inhomogeneity in the spin, charge and lattice of cuprates, using neutron and NMR spectroscopies.

Program Impact: Program is recognized internationally for its leadership in creating new science through discoveries of new correlated electron materials.

Interactions: Z. Fisk (now at Florida State University), H. R. Ott (ETH Zurich), I. K. Schuller and F. Hellman (U.C. San Diego), D. E. MacLaughlin (U.C. Riverside), G. Aeppli (NEC), B. Buchner (University Cologne), C. Retorri (UNICAMP), J. Lawrence (U.C. Irvine)

Recognitions, Honors and Awards (at least partially attributable to support under this FWP or subtask): Z. Fisk-National Academy of Science, American Academy of Arts and Sciences, E. O. Lawrence Prize, DOE Award for Sustained Outstanding Research in Solid State Physics, APS New Materials Prize, APS Fellow, APS Div. Condens. Matt. Phys. Executive Committee, APS Buckley Prize Committee, LANL Fellow, editorial boards of Physica B and Phys. Rev. Lett.; P. C. Hammel-APS Fellow, LANL Fellow, LANL Fellows' Prize, APS Executive Committee of Instrumentation and Measurement Science; R. H. Heffner-APS Fellow; R. McQueeney-Caltech Visiting Scientist; R. Pynn-APS Fellow, AAAS Fellow; J. L. Smith- E. O. Lawrence Prize, DOE Award for Sustained Outstanding Research in Solid State Physics, APS New Materials Prize, APS Fellow, LANL Fellow, editorial boards of J. Alloys and Compds. and Phil. Mag.; J. D. Thompson- APS Fellow, APS Div. Condens. Matt. Phys. Executive Committee, DOE Award for Sustained Outstanding Research in Solid State Physics, ISI Highly Cited Physicist, LANL Fellow, LANL Fellows' Prize, Japanese Society for the Promotion of Science Fellow

Personnel Commitments for FY2002 to Nearest +/-10%: J. D. Thompson (20%), W. Bao (40%), M. Fitzsimmons (40%), R. H. Heffner (15%), R. McQueeney (40%), R. Movshovich (20%), J. L. Sarrao (20%), five postdocs (75%)

Authorized Budget (BA) for FY00, FY01, FY02
FY00 BA $1,374,000 **FY01 BA** $1,235,000 **FY02 BA** $1,266,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0202020

FWP and possible subtask under FWP:
Photoelectron Spectroscopy of Transuranics

FWP Number: 04SCPE437

Program Scope: The electronic structure of actinide elements and compounds is investigated via photoelectron spectroscopy using both a novel laser plasma light source (LPLS) which is tunable between 27eV and 140 eV photon energy, as well as synchrotron radiation whenever possible. The LPLS uses a continuous-flow mercury target and a high power Nd:YAG laser to provide a tunable source of photons for photoelectron spectroscopy over the ultraviolet and soft x-ray energy range, encompasses the 5f resonant photon energies and regions of maximum change and intensity in 5f electron cross-section. This is essentially the capability of a synchrotron without the associated public transuranic risks, albeit at reduced intensities. Surfaces are prepared via laser ablation, allowing for cleaning at low temperatures. Laser ablation is demonstrably the best method for preparation of transuranic surfaces in PES measurements. Both α- and δ-Pu display a sharp density-of-states near the Fermi energy, indicative of narrow bands, but neither fits the usual heavy fermion picture. From the cross section dependence we deduce a substantial 6d admixture in these bands. Angle resolved synchrotron work on uranium compound single crystals reveals definite 5f-6d hybridized bands, somewhat renormalized from calculated bands, even for cases of ordered magnetic moments. It now appears that the correct description of 5f-electron materials through Pu and its compounds is narrow band behavior very near the Fermi energy if the 5f electrons are not clearly localized in a magnetic configuration. In most cases including 4f systems, the f-electrons are confined to only part of reciprocal space. Photoemission measurements have now been made on single crystal U compounds (synchrotron), Np compounds (NpAs, NpSb, NpTe - LPLS) and Pu compounds ($PuIn_3$, $PuSb_2$, $PuCoGa_5$, $PuSn_3$, PuTe, PuSb - LPLS) with six different Pu compounds measured in the last 18 months.

Major Program Achievements (over duration of support):
Tie between surface energies, work function and PES measurements (J. Chem Phys. 278, 111 (2002)).
Angle-resolved PES in 4f and 5f electron materials (JESRP 117, 323 (2001)).
Direct comparison between PES and calculations for α and δ-Pu (PRB 62, 1773 (2000)).
First measurement for NpAs hybridization and 5f bands (Los Alamos Science 26, 120 (2000)).
Demonstration of band behavior for actinide f-electrons (Gschneidner Handbook, Chap. 172 (1999)).
First resonance photoemission data on Pu metal (Surf. and Interface Analysis 26, 121 (1998)).
LPLS design and laser ablation for cleaning transuranics (J. Alloy & Comp. 286, 14 (1999)).

Interactions: external collaborators include G. Lander (Karlsruhe), C.G. Olson (Ames Lab), H. Hochst (Univ. of Wisconsin), P. Riseborough (Temple), M. Jarrell (Univ. of Cincinnati), G. Kotliar (Rutgers), F. Wastin (Karlsruhe), internal collaborators include L. Morales (NMT-16), John Wills (T-1).

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
A.J Arko elected Fellow of Los Alamos National Lab. J.J. Joyce elected to advisory committee of Synchrotron Radition Center and serves on the local arrangements committee 61^{st} Physical Electronic Conference. Arko and Joyce have had 20 invited talks and 23 publications (1998 to 2002) including 1 book chapter with over 50 publications since program inception in 1992.

Personnel Commitments for FY2002 to Nearest +/-10%:
J.J Joyce, .30
A.J. Arko, .25
Martin T. Butterfield, (Postdoc) .50
Tomasz Durakiewicz, (Postdoc) .50
Elzbieta (Ela) Guziewics, (Postdoc) .50.

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $392, 000 **FY01 BA** $353,000 **FY02 BA** $300,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0202030

FWP and possible subtask under FWP:
Magnet Project

FWP Number: 04WCPE438

Program Scope: This program establishes a DOE user research facility and a Magnet Access Team (MAT) whose centerpiece is a 100 tesla multi-shot (100T-MS) magnet at the National High Magnetic Field Laboratory in Los Alamos. At all magnetic fields above 80 teslas, this magnet will be unique in the world. Materials research in which very high magnetic fields prove invaluable include, for example, studies of high temperature superconductors, correlated electron phenomena, fermiology, magnetic anisotropy and exchange in rare-earth and transition-metal compounds, field-induced magnetic and electronic phase transitions, transport in quantum-confined systems, magneto-optical effects in nano-dots. Magnetic fields also provide a litmus test of competing theories of the phase diagram of plutonium. Higher magnetic fields translate into a larger energy scale with which the electronic structure of materials can be probed. At 100 tesla the energy scale approaches the energy scale of the orbital, spin and coherence energy scales of many compounds, as well as the thermal energy at room temperature. This enables 100 tesla magnetic fields to probe or manipulate phenomena first observed near room temperature.

Major Program Achievements (over duration of support):
Construction has begun on the magnet. The coil vendor is now inspecting the fabricated conductor. Winding outer coils will commence in early 2003. Busbar analysis and modeling are complete. Busbar and support structure drawings, as well as frame plate structure modeling are almost complete. The dewar has been delivered to LANL. Insert Capacitor Bank assembly is underway, along with design and fabrication of two types of insert prototypes. Most of the reinforcing shells are forged and delivered to coil vendor for fabricating nano-structured sheet wound shell structures. Apparatus for proof testing a prototype 100T sheet-wound shell at operating temperatures is being designed. Magnet assembly is slated to begin in the third quarter of 2003 with testing of the magnet to commence in late 3rd quarter or early 4th quarter of 2004. Work to develop experimental techniques for use on the 100T-MS magnet has resulted in a series of publications which demonstrate advances in magneto-transport and ultrasound techniques in the pulsed magnetic field environment, including a 2002 article in Nature magazine.

Program impact: Development of high performance conductors with high strength, ductility and ; Innovative high strength magnet coil designs with high performance materials (cold-worked 301 stainless steel and MP35N) and deliberate autofrettage to realize beneficial pre-stressing; Development of ultrasensitive micromachined magnetometer; Discovered metal-insulator crossover in La-doped BSCO cuprates; Development of megagauss sensors based upon linear magnetoresistance in silver chalcogenides; Development of unique ultrasensitive Hall measurements in pulsed magnetic fields, applied to studies of high-Tc cuprates; Development of ultrasound techniques for magnetic field experiments across the charge-density-wave transition in monocrystal Lu5Ir4Si10; and the metamagnetic transition in URu2Si2; Formation of a world-leading team of experimentalists developing advanced instrumentation for static and pulsed fields

Interactions: Collaboration with R. Hoagland and D. Embury on metallurgy; significant external collaborators include L. Li, Y. Eyssa, and K. Han (Florida State University) on magnet design; Y. Ando, S. Ono (CRIEPI, Tokyo) on high-Tc experiments; T. Rosenbaum (U. Chicago) on silver chalcogenide experiments. Materials collaborations with OMG Americas (GlidCop precursor rod), Handy & Harmon (copper silver ingots), Teledyne Wah Chang (hot rotary forging of CuAg ingots), IGC-Advanced Superconductors (drawing of GlidCop and CuAg conductors), Allegheny Ludlum (High strength 301 SS sheet) and CSM Industries (MP35N strip) and Everson (coil fabrication).

Recognitions, Honors and Awards: A. Migliori (Fellow, APS 2000); G. Boebinger: Five public outreach lectures on “Levitation, Superconductivity and the World’s Largest Magnets”, LANL Frontiers of Science Lectures (2002).

Personnel Commitments for FY2003: (% FTE paid from this grant given in parentheses) **Science Team:** A. Migliori (team leader) 50%, (0% paid from this grant), G. Boebinger 10% (0%), F. Balakirev 40% (0%), J. Betts 60% (30%). Engineering team: J. Sims (team leader) 20% (10%), J. Schillig 40% (0%), G. Ellis (35%), J. Bacon (50%), C. Ammerman (30%), K. Kihara (25%), K. Hurtle (20%), Three technicians, 50% each (0% from this grant).

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $836,000 **FY01 BA** $787,000 **FY02 BA** $700,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC020102

FWP and possible subtask under FWP:
Equilibrium and Non-equilibrium Statistical Mechanics of Dislocations

FWP Number: 04SCPE493

Program Scope: A combination of computer simulation and theoretical analysis is being used to develop the equilibrium and non-equilibrium statistical mechanics of evolving dislocation microstructures. The goal is to use statistical mechanics to find a correct homogenization of variables to reduce them to what is minimally needed to describe the mechanical behavior. We are first developing a framework for a density-functional theory of dislocation structures, based on the continuous dislocation density tensor. Comparing results from the continuous dislocation scale with simulations based on discrete dislocations, our focus throughout will be the identification of the critical variables needed to describe structure and dynamics. This work is a necessary step for developing a fundamental theory to bridge the gap between the complex dislocation microstructures and macroscopic response.

Major Program Achievements (over duration of support):
We have identified a free energy functional for dislocations in terms of the continuous dislocation density. We have shown that the long-range part of the interaction can be treated with a simple multipole expansion of the density functional and have identified two approaches for addressing the short-range behavior, both of which are under further investigation.
We have derived an analytical expression for how temperature-induced fluctuations in the dislocation lines modify the interaction between parallel screw dislocations.
We have derived analytical expressions for the effects of solutes on dislocation motion, identifying distinct regimes of behavior. We showed that one can model the effects of solutes without explicitly treating the solute degrees of freedom, enabling possible simplifications in future simulations of dislocation systems that include solutes.

Program Impact:
The work to date provides a framework for incorporating dislocation substructure in the continuous theory of dislocations. This advance is a first step in developing a course-grained theory of dislocation behavior.

Interactions:
Lehigh University: Materials Science and Engineering (J. Rickman)
Princeton University: Mechanical and Aerospace Engineering (D. Srolovitz)
Florida State University: School of Computational Science and Information Technology (J. Viñals)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
R. LeSar: 6 Invited talks since 2001; Editor: Computational Materials Science; Adjunct Professor of Materials Science and Engineering: University of California, Santa Barbara; Chair, Gordon Conference on Physical Metallurgy, 2004.

Personnel Commitments for FY2002 to Nearest +/-10%:
R. LeSar 65%
J. Lewis (student) 25%

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $300,000 **FY01 BA** $276,000 **FY02 BA** $270,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0201020

FWP and possible subtask under FWP:
Ensemble-Controlled Deformation Behavior in Materials

FWP Number: 04SCWE401

Program Scope: Our primary goal is to use experiment and modeling to characterize and predict the complex and collective response of the evolution of ensembles of defects in materials during plastic deformation. Defects, in this context, include point defects, dislocations, twins and grain boundaries, and thus span many length scales. The deeper significance of the proposed work will be the development of the connection between the neighborhood-based descriptions of the defect ensembles at length scales spanning from atomistic to continuum to the overall mechanical response of a material. This new program (started during FY'01) was a result of restructuring three older programs: (E413- Mechanical properties, E415- Evolving microstructures, E430- High temperature materials). The achievements listed below reflect the combined effort of work in E413, E415, E430 and E401 over the history of these programs.

Major Program Achievements (over duration of support): One thrust of this program was to understand and account for the role that crystallographic texture plays in the mechanical response and the anisotropy of polycrystal aggregates (most metallic systems). A book was published ("Texture and Anisotropy", U.F. Kocks, C.N. Tomé and R.H. Wenk, Cambridge University Press, Cambridge, England, 1998) which summarizes the achievements of this portion of the program.
Another thrust was to develop constitutive equations describing the mechanical response of cubic materials, under a wide range of strain, temperature and strain-rate regimes. This resulted in the Mechanical Threshold Strength model, which is now widely used in Los Alamos and also in other research institutions worldwide.

Program impact: The effort on textures, anisotropy, constitutive description and modeling of polycrystal plasticity came at the time when the Materials Science community started becoming aware of these issues. It changed the way in which constitutive modeling was approached not only at Los Alamos, but also throughout the scientific community as well. Los Alamos can be regarded as playing a major role in installing such issues in the community. The work done on this program had an impact on the way dislocation simulations are performed at Los Alamos and elsewhere by introducing methods to appropriately treat long-range forces and by showing how a commonly used truncation method could lead to incorrect results. This program also developed one of the first and clearest examples of a transition between the behavior of discrete dislocations and continuum response of a material in examining the dynamic development of plastic zones in front of a crack.

Interactions: H.-R. Wenk (UCB), R.A. Lebensohn (U. of Rosario—Argentina), P. Dawson (Cornell U.), A. J. Beaudoin (U of IL—Urbana), S. R. MacEwen (ALCAN), S. I. Wright (TexSEM Labs), J. M. Rickman (Lehigh U.), David J. Srolovitz (Princeton Un.), Darcy Hughes (SNL CA), Phillip Duxbury (Michigan State Un.), M. Miodownik (Kings Col. London), A. King (Purdue U.), R. W. Grimes (Imperial Col.), A. H. Heuer (CWRU), J.P. Hirth.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP):
U. Fred Kocks, Fellow, (99 NAE, 87 TMS, LANL, ASM, APS, AIME); Sig Hecker, LANL Senior Fellow, Mem. NAE; Fellow (AAAS, ASM, TMS), DOE, E.O. Lawrence Award, (1984), DOE Dist. Ass. Award, (1997); K.B. Alexander, Fellow, (ASM, ACS); T.E. Mitchell, Fellow (LANL, TMS, ASM, APS, ACS), Honorary D. Sc., U. of Cambridge; Symp. and special issue of Phil. Mag. A in his honor; S. A. Maloy, *Robert Lansing Hardy Prize of the Metals, MMS* (1998); J.J. Petrovic, Fellow (LANL, ACS, ASM); M.I. Baskes, Fellow, IP, DOE BES Award for Sustained Outstanding Res: *Dev. of the Embedded Atom Method* & *Atom. Studies of Helium in Metals,* Journal Editor, *Modeling and Sim. in Materials Sci. and Eng.;* E.A. Holm, Fellow, ASM; R. LeSar, Ass. Western Univ. DOE Dist. Lecturer and Journal Editor, *Com. Mat. Sci.*

Personnel Commitments for FY2002 to Nearest +/- 10%:
K.B. Alexander (10%, till Dec'01), M.I. Baskes (25%), A. Misra (20%), C.N. Tomé (25%), I. Beyerlein (20%), G.C. Kaschner (40%), R. A. LeSar (25%), S. Swaminraryan (40%), S.G. Srivilliputhur (25%), M.G. Stout (20%), T. E. Mitchell (20%), R. McCabe (100%, post-doc), S. Mahesh (100%, post-doc), Z. Wang (GRA, UCLA, summer).

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $1,049,000 **FY01 BA** $1,142.00 **FY02 BA** $1,072,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0201050

FWP and possible subtask under FWP:
Ion-Enhanced Synthesis of Materials

FWP Number: 04SCWE407

Program Scope: To develop a fundamental understanding of ion and plasma processed materials and to determine how ion and plasma processing parameters influence the material structure and functional properties. Experiments, theory and modeling are used to understand the underlying physics and fundamental processes responsible for the enhanced properties derived by materials synthesis by these methods.

Major Program Achievements (over duration of support): We have successfully developed the Plasma Immersion Ion Process (PIIP) to synthesis diamond-like-carbon (DLC) field emitters. Modeling showed that electron emission is dependent sp^3 contents and the aspect ratio of the emitting area. PIIP was then used to alter the surface topology and ratio of sp^2 to sp^3 carbon bonding at the surface and thereby control the electron emission behavior.

A novel approached for synthesizing highly adherent hydroxyapatite coatings on titanium prosthetic devices such as hip, knee and dental implants, was developed using a combination of ion-beam intermixing between a sol-gel-based (note hyphen) coating and the titanium. This synthesis method relied on intermixing that occurs in collision cascades and plasma-ion implantation for treating prosthetic devices of any shape. This approach is capable of tailoring the hydroxyapatite's outer surface to promote easy bone growth thus reducing the risk of implant failure

We have shown that the intrinsic stress in thin films form by ion assisted deposition techniques are strongly influence by the presence of grain boundaries, vacancies, interstitials and dislocations. An atomic interaction model has been developed to explain the source of intrinsic stress in thin films.

We have shown for the first time that the radiation defects produced during the ion implantation of hydrogen into silicon promotes the formation of hydrogen-planner defects. A critical component in the formation of these hydrogen-planner defects is the in-plane biaxial compressive stress distribution that results directly defects produced during ion implantation. A direct consequence of the biaxial compressive stress field is a corresponding out-of-plane tensile strain distribution that mirrors the radiation defect profile. Staining the lattice reducing the energy needed to place hydrogen at bond centered sites between adjacent silicon atoms thereby facilitating the nucleation and growth of hydrogen platelets on planes normal to the ion implantation direction

Program impact: Provides fundamental insight at the microscopic and atomistic levels on how ion-solid interactions enhance the properties and functionality of materials. This work has enabled the synthesis of novel and improved materials.

Interactions: J. C. Barbour (SNL-NM), A. Haynes (ORNL), O. W. Holland (ORNL), J. Mayer (ASU), S. S. Lau (UCSD), M. Masquelier (Motorola), L. C. Feldman (Vanderbilt Univ.), S. Barnett (Northwestern Univ.), F. Rossi (Joint Research Center, Ispra, Italy), D. Lucca (Oklahoma State); *Internal LANL*: M. G. Tuszewski, H. Kung, A. Misra, M. Baskes, R. Schwarz.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
M. Nastasi: Fellow of LANL (2000), Recipient LANL Fellows Prize (1995), R&D 100 Award (1997), Exec. Officer of The Bohmische Physical Society (1997-), Edit. Board of Nuclear Instruments and Methods in Physics Research, Section B: (1997-), Principal Ed. J. of Materials Research (1997-2000), Chair MRS Bull Pubs Subcommittee (1994-1999), Chair of the Editorial Board of MRS Bull (1996-1999), *Adjunct Professor*, Univ. of Colorado, Arizona State Univ., Univ. of Maryland.

Personnel Commitments for FY2002 to Nearest +/- 10%: M. Nastasi (PI) 40%, B. Taylor (tech) 60%, G. Swadener (TSM) 20%, I. Afanasyev (postdoc) 100%, L. Jacobsohn (postdoc) 100%

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $584,000 **FY01 BA** $510,000 **FY02 BA** $547,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC020601

FWP and possible subtask under FWP:
Active Assembly of Dynamic and Adaptive Materials

FWP Number: 04SCPE953

Program Scope: Understanding and controlling the coupling and interplay of *dynamic assembly* and *active transport* to assemble complex, functional structures in artificial environments; employing either *programmed* or *adaptive* modes; using biological and artificial nano-scale components. Develop new paradigm in which nano-building blocks are assembled and reconfigured into desired structures in response to external stimuli; mimicking biological systems. Combine experimental results with computer-based modeling of the scaling laws of energy consumption in living systems; develop optimal structural organization required to achieve efficient energy usage and input.

Major Program Achievements (over duration of support): The project started in the last quarter of FY02.

Program impact: The project started in the last quarter of FY02.

Interactions: The project started in the last quarter of FY02.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): The project started in the last quarter of FY02.

Personnel Commitments for FY2002 to Nearest +/- 10%:
The project started in the last quarter of FY02.

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $ 0.00 **FY01 BA** $0.00 **FY02 BA** $100,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0202020

FWP and possible subtask under FWP:
Thermal Physics

FWP Number: 04SCWE426

Program Scope: We study fundamental principles of thermal physics and their application in science and technology. Specifically, we explore novel concepts in heat engines, especially thermoacoustics, with an emphasis on establishing scientific foundations for new technologically useful energy-conversion devices. We also study fundamental concepts of nonlinear physics and statistical mechanics in fluids and granular media.

Major Program Achievements (since 1981):

Invention and demonstration of thermoacoustic refrigeration. Creation of efficient thermoacoustic engine (with 25% of Carnot efficiency). Invention and demonstration of thermoacoustic-Stirling hydrid heat engine (with 40% of Carnot efficiency). Discovery of thermoacoustic mixture separation. Demonstration of useful thermoacoustic cooling using steadily flowing process gas as acoustic gas. Invention and demonstration of superfluid Stirling and superfluid orifice pulse-tube refrigerators. Development of physical acoustics principles underlying all of the above.

Experimental demonstration of early concepts of chaotic nonlinear dynamics, specifically quasiperiodicity and mode locking. Discovery of novel states of rotating convection and anomalous scaling of pattern dynamics. First measurements of heat transport scaling in rotating turbulent convection. Demonstration of sensitive dependence of spatially extended system to local disturbances. Application of statistical mechanics to granular chain dynamics and unknotting phenomena.

Program impact: Natural-gas liquefier CRADA with Praxair Inc. (funded in part by DOE/Fossil and NIST ATP). Thermoacoustics textbook and design software are used worldwide. Academic thermoacoustic groups worldwide owe their roots to this program. On the organizing committees of 11 international conferences. Invited speakers at a few international conferences per year, with 7 invited talks at APS meetings. Approximately 200 refereed publications including 19 in Phys. Rev. Lett., 1 in Science, and 2 in Nature. Approximately 20 patents. Support of 20 postdocs who have gone on to great things elsewhere in academic, industrial, and government research.

Interactions: Natural-gas liquefier CRADA with Praxair Inc. (funded in part by DOE/Fossil and NIST ATP). Los Alamos Center for Nonlinear Studies.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP): <u>Ecke</u>: Fellow of Los Alamos National Laboratory, Chair (2001) APS Topical Group on Statistical and Nonlinear Physics, APS Division of Fluid Dynamics Nominating and Fellowship Committees, Editorial Board of Chaos; <u>Swift</u>: Fellow of Los Alamos National Laboratory, Fellow of the American Physical Society, Fellow of the Acoustical Society of America, Silver Medal in Physical Acoustics of the Acoustical Society of America; <u>Swift et al.</u>: Two R&D100 Awards: Coolahoop, and Acoustic Stirling Heat Engine; <u>Backhaus</u>: Los Alamos Postdoctoral Prize in Experimental Physics, Reines Fellowship.

Personnel Commitments for FY2002 to Nearest +/- 10%: G. W. Swift 50%, R. E. Ecke 20%, D. L. Gardner 10%, postdoc D. A. Geller 100%, technician C. N. Espinoza 50%.

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $566,000 **FY01 BA** $540,000 **FY02 BA** $439,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0203010

FWP and possible subtask under FWP:
Electronic Devices from Nanocell Organics Crystals

FWP Number: 04SCPE950

Program Scope: This project is part of the NSET program. The goal of the project is to provide the fundamental scientific underpinnings for the behavior of organic semiconductors devices including field effect and light emitting devices. To do this we focus primarily on single crystals where the defect density is significantly lower than that in amorphous or polycrystalline films. The main activities of the project are 1) Developing the expertise in organic crystal growth. 2) Developing the capability for deposition of electronic device elements on soft materials, such as van der Waals bonded organic crystals. 3) Elucidating the optical response of such materials including time-domain methods, as well as equilibrium photo-doping studies.

Major Program Achievements (over duration of support):
•Over the past year, we have built a laboratory for the synthesis of organic crystals, the fabrication of devices made from such crystals, and the semiconductor measurements used to extract physical parameters for device performance. The crystal synthesis apparatus includes several vapor-transport furnaces and two potentiostats, the latter for growth of charge-transfer salts. For device fabrication and testing we have set up two thermal evaporation systems, two rf-magnetron sputterers, and a general purpose cryostat with electronics for measuring electronic transport.
•We have successfully synthesized a number of organic compounds, including the polyacenes (pentacene ($C_{22}H_{14}$), tetracene ($C_{18}H_{12}$)), ET ($C_{10}H_8S_8$), Coronene ($C_{24}H_{12}$), TCNQ ($C_{12}H_4N_4$), and performed nonlinear conductivity measurements.
•We have made gated FET structures from both pentacene and C_{60} using equipment purchased from the NSET grant and with crystals grown with NSET funds. These devices have on/off ratios as large as 10^6 at a gate voltage of 30 volts operating at room temperature. These are among the first such structures to be made from single crystals.
•We have performed extensive characterization of the trapping behavior in pentacene, C_{60}, tetracene, ET and other compounds. We have found large variability of the current-voltage properties from sample-to-sample. This variability can be minimized, and the effective two-wire resistance lowered by annealing in forming gas. For C_{60}, the trapping density of states is extremely narrow, leading to two different types of trapping behavior associated with orientational ordering at 260K.

Program Impact:
This project has produced some of the first results for devices made from single crystals. It is expected that from this work, fundamental limits on organic device performance can be understood. This will enable the development of faster organic devices, and ones with higher efficiency for light conversion.

Interactions:
University of California, Santa Barbara: Physics (A. Heeger)
University of California, Riverside (R. Haddon)
University of California, Berkeley (J. Orenstein)
Bell Labs, Lucent Technologies (C. Kloc)
Stanford University (Z-X. Shen)
Johns Hopkins University (C. Broholm)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
The project started in FY02.

Personnel Commitments for FY2002 to Nearest +/-10%:
A. P. Ramirez (group leader) 50%
V. Butko (TSM) 30%
X. Chi (postdoc) 100%
V. Thorsmiele (postdoc) 100%

Authorized Budget (BA) for FY00, FY01, FY02:
FY01 BA $0 **FY02 BA** $100,000 **FY03 BA** $650,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0203010

FWP and possible subtask under FWP:
Macromolecular Assemblies; Cooperative Phenomena in Molecular Nanocomposites.

FWP Number:
04SCPE585; 04SCPE896

Program Scope:
The goal of this research is to explore the structure and dynamics of complex fluid assemblies, organic-inorganic hybrids and composites, and biomimetic materials over several orders of length and time scales. Expertise in sample preparation and characterization, neutron scattering, and theoretical modeling and simulation are applied in an integrated manner to gain new insights into the balance between forces that govern the organization and responses of the materials studied. In part, the project has arisen from the restructuring of previous projects on organic and inorganic macromolecular electronic systems and neutron scattering studies of chemical materials.

Major Program Achievements (over duration of support):
Provided definitive proof of the nature of the chemical bond between dihydrogen ligands and metal centers (using inelastic neutron scattering studies of dihydrogen rotation), as well as elucidation of the electronic factors that govern stable dihydrogen bonding. Made the first direct observation of proton transfer in dihydrogen-hydride exchange by quasielastic neutron scattering. Provided clarification of possible physical mechanisms involved in long-range energy transfer in crystalline peptide H-bonded systems (proteins), pointing towards vibrational polarons as most likely. Developed many-body theory and simulations, validated with an extended set of synthetic and experimental studies, that described a class of quasi-one-dimensional charge transfer complexes, including an understanding of tunable broken-symmetry ground states and collective excitations. Demonstrated multi-quanta bound states as an intrinsic energy localization mechanism in polarizable electronic materials with strong electron-lattice coupling. Development and use of neutron confinement cell. Modeling, simulation and spectroscopic characterization of polyelectrolytes, two-component lipid mixtures, layered organic/inorganic hybrid crystalline materials, and surfactant/silica mesophase composite materials. Masked photolytic removal of organic phase in organic/inorganic nanocomposite materials to generate patterned functionalities in thin-films.

Program impact:
Development and characterization of substrate- and polymer-supported phospholipid membrane assemblies with uses in biotechnology applications; Combined experimental and theoretical description of electronic, vibrational and structural responses of classes of chemically tuned low-dimensional polymeric and crystalline materials with impact on optimization of electronic devices; Development of photolytic methods for organic template removal in organic/inorganic composite materials with potential impact in sensor development and catalysis.

Interactions:
A.K. Cheetham (UC Santa Barbara); H. Fehske (Univ. Bayreuth); J. Israelachvili (UC Santa Barbara); C. Safinya (UC Santa Barbara); S.L. Dexheimer (Washington State University); A.N. Parikh (U.C. Davis); T. Kuhl (UC Davis); M. Barthes (U. de Montpellier); A. Heeger (through 1994); A. McDiarmid (through 1992).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Department of Energy E.O. Lawrence Award (A.R. Bishop, 1993); Senior Humboldt Fellow (A.R. Bishop, 2000); First recipient of LANSCE Director's Award for Scientific Excellence (G. Smith, 2000); Symposium Organizer for Spatially Resolved Characterization of Local Phenomena in Materials and Nanostructures, Materials Research Society Fall 2002 meeting (A. Shreve, 2002); Symposium Organizer for Filled and Nanocomposite Materials, Materials Research Society Fall 2000 meeting (R. Hjelm, 2000).

Personnel Commitments for FY2002 to Nearest +/- 10%:
G. Smith (10%); R. Hjelm (20%); J. Majewski (10%); A. Shreve (10%); J. Eckert (20%); T. Lookman (10%); A. Dattelbaum (postdoc 100%); M. Amweg (student 100%).

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $744,000 **FY01 BA** $690,800 **FY02 BA** $623,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0203010

FWP and possible subtask under FWP:
Macromolecular Assemblies; Cooperative Phenomena in Molecular Nanocomposites.

FWP Number: 04SCPE951

Program Scope:
This project aims at developing self-assembly and biomolecular-assisted assembly methods to create complex functional nanoscale materials capable of long-lived photo-induced charge separated states. The research program is designed to address the goals of understanding the properties of electronically active molecular and macromolecular building blocks that can be incorporated into self-assembled materials, of developing self-assembly and biologically assisted assembly methods to create multicomponent electronically active materials from the relevant building blocks, and of combining experimental and theoretical studies of the structure, dynamics, efficiency and mechanisms of charge transfer functions in the assembled materials.

Major Program Achievements (over duration of support):
This new program has been funded only since August 2002 (approximately 2 months).

Program impact:
The program is expected to impact the understanding of how to control complex self assembly to create functional nanoscale materials. Applications of such materials are found in energy production and storage, catalysis, and sensor technologies.

Interactions:
A.N. Parikh (U.C. Davis); J.A. Brozik (U. New Mexico); D. Evans (U. New Mexico); V. S-Y Lin (Iowa State University); D. Sasaki, J. Shelnutt (Sandia National Laboratory).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Not applicable (funding initiated at end of FY2002).

Personnel Commitments for FY2002 to Nearest +/- 10%:
Not applicable (funding initiated at end of FY2002).

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $0.00 **FY01 BA** $0.00 **FY02 BA** $750,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0201020

FWP and possible subtask under FWP:
Neutron Irradiation Induced Metastable Structures

FWP Number: 04SCPE429

Program Scope: The goal of this program is to understand the radiation damage response of ceramics exposed to neutrons or other energetic particles. Our studies of the damage response of ceramics address two objectives: (1) to predict microstructural evolution in ceramics exposed to radiation; and (2) to identify the physical aspects of ceramics that are effective in promoting radiation resistance. Our ultimate goal is to design new radiation resistant ceramics. We conduct particle irradiation tests on ceramics to evaluate their irradiation damage response. We also perform computer simulations of damage evolution in ceramics to assist in our understanding of radiation damage phenomena in these materials. Our research is focused on highly radiation-resistant ceramics. We have determined that damage accumulation in oxides such as $MgAl_2O_4$ and ZrO_2 occurs at far lower rates than in most other ceramic oxides. We expect radiation tolerant ceramics to find application in existing fission reactors, in future fusion reactors or accelerator-based reactors, or as actinide-host ceramic fuelforms and wasteforms.

Major Program Achievements (over duration of support): Using atomistic computer simulation techniques along with ion beam irradiation experiments on selected oxides, we have demonstrated that a group of compounds with chemical formulae given by $A_2B_2O_7$ and with crystal structures similar to that of the mineral fluorite are highly resistant to displacive radiation damage. Our findings suggest that a large number of isochemical $A_2B_2O_7$ compounds with a structure called pyrochlore (very similar to the fluorite structure, but more highly ordered) should not exhibit resistance to radiation damage. Many of the $A_2B_2O_7$ compounds with the fluorite structure should be suitable hosts for actinide species (Th, U, Pu, etc.) as well as other radiotoxic nuclides including fission products. This research has been published in Science: K. E. Sickafus, L. Minervini, R. W. Grimes, J. A. Valdez, M. Ishimaru, F. Li, K. J. McClellan and T. Hartmann, "Radiation tolerance of complex oxides," Science **289** (2000) 748-751.

Program Impact: Early work on this program laid the foundation for our current understanding of the behavior of model ceramic oxides (such as periclase (MgO) and corundum (Al_2O_3)) in a radiation damage environment. Recent developments on this program have led to an exciting new predictive capability to assess the radiation tolerance of oxides with very complex chemistries and structures (examples include $A_2B_2O_7$ pyrochlores and fluorites). Other efforts: Mike Nastasi co-instructed an MRS Short Course entitled "Fundamentals and Applications of Ion Beam Processing" in Boston MA (1990). Mike Nastasi organized the Tenth International Conference on Ion Beam Modification of Materials, held in Albuquerque, NM (1996). Kurt Sickafus organized an international symposium on "Spinel Compounds: Structure Property Relations" at the Annual Meeting of the American Ceramic Society, Cincinatti, OH (1998). The proceedings was published as a special topical issue of the Journal of the American Ceramic Society (Vol. 82(12) 1999).

Interactions: R. W. Grimes (Imperial College); Hj. Matzke (Institute for Transuranic Elements, Karlsruhe, GERMANY); V. T. Gritsyna (Kharkiv State University, Kharkiv, UKRAINE). [In August, 2000, Gritsyna and Sickafus were awarded a collaborative research grant from the United States Civilian Research and Development Foundation (CRDF) entitled "Spatial Distribution and Interaction of Defects in Magnesium Aluminate Spinel, Based on Kinetic Studies of Irradiation Induced Processes Using Optical Methods."]. *Internal LANL Interactions*: Ken McClellan, Steve Valone, Marius Stan, Chris Wetteland, Mike Nastasi, and Mike Baskes.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Fellow of the American Ceramic Society to Frank Clinard (1986), Foreign Distinguished Visiting Scientist at JAERI, Tokai, JAPAN to Frank Clinard (1987), LANL Fellow's Prize to Mike Nastasi (1995), Fellow of the American Ceramic Society to Kurt Sickafus (1998), Fellow of Los Alamos National Laboratory to Mike Nastasi (2000), LANL Fellow's Prize to Kurt Sickafus (2001), 2002 OBES Chunky Bullet competition co-winner (2002).

Personnel Commitments for FY2002 to Nearest +/-10%:
K. Sickafus, Staff 100%; J. Valdez, Tech 100%; M. Tang, GRA, NM Tech. 100%; A. Cleave, GRA, Imp. Col. 100%

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $555,000 **FY01 BA** $557,000 **FY02 BA** $646,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0201020

FWP and possible subtask under FWP:
Science of Electronic and Optical Interactions between Coupled Nanostructures

FWP Number: 04SCPE395

Program Scope:
The goal of this project is the understanding of the behavior of interacting nanophotonic and nanoelectronic structures. One focus area is the interactions that produce changes in the optical and electronic properties of the nanostructures. We are investigating the effect of inter-dot interactions on the optical and electronic properties of self-assembled and colloidal quantum dot arrays. The second activity will be an exploration of novel composite materials consisting of semiconductor colloidal quantum dots embedded in Inorganic and organic semiconductors. A second focus area is the study of nanoelectronic structures in photonic bandgap materials and photonic crystal fibers. The interplay between the restricted electronic density of states and the restricted photonic density of states can produce large optical nonlinearities, can inhibit radiative decay, producing "photon bound states", and can perhaps lead to high speed optical switching

Major Program Achievements (over duration of support):
We performed time- and spectrally resolved studies of resonant energy transfer in monodisperse, mixed-size, and layered assemblies of CdSe nanocrystal quantum dots. These studies reveal time, size, and energy scales for energy transfer and suggest routes toward engineered design of quantum-dot assemblies for light harvesting and directed energy flow.
In photonic crystal fibers (PCFs), the phase and amplitude signatures of ultrafast pulse propagation in the soliton and the Raman self-frequency shift regime were characterized for the first time. These pulses are a source of tunable femtosecond pulses in the mid infrared wavelength range. We also observed in PCfs polarization controlled third harmonic generation of both the input pulse and the Raman self-shifted pulse.
Theoretically, we investigated the ground state properties of ferromagnetic metal/conjugated polymer interfaces to understand electron charge and spin transfer from the ferromagnetic metal to the organic polymer, and structural relaxation near the interface.

Program impact:
This project addresses important scientific issues at the forefront of nanoscience. It is vitally connected to the joint Sandia/Los Alamos Center for Integrated Nanotechnologies (CINT). The portfolio of activities contained within this program will unify nanoelectronics and nanophotonics research at Sandia and Los Alamos, further establishing a firm foundation of ongoing nanoscience relevant to CINT.

Interactions:
Department of Physics, University of Bath, UK; Department of Physics, University of Florida, Gainesville; Center for High Technology Materials, University of New Mexico; Department of Physics, University of Puebla, Mexico; Department of Electrical Engineering, Oklahoma State University; Naval Research Lab; Department of Chemistry, MIT; Department of Physics and Astronomy, Georgia State University

Recognitions, Honors and Awards (at least partly attributable to support under this FWP):
V.I. Klimov—7 invited talks in FY02
A. J. Taylor -- Fellow of the American Physical Society, (2002), Fellow of the Optical Society of America, (2002), Topical Editor, Journal of the Optical Society B, Director-at-Large Optical Society of America, 2002-2005, Program Cochair, APS Laser Science XVIII Conference, 2002, 7 invited talks in FY02.

Personnel Commitments for FY2002 to Nearest +/- 10%:
Staff: A. J. Taylor, 10%, V.I. Klimov, 10%, D. L. Smith, 20%
Postdocs: M. Achermann, 50%, A. Efimov, 50%

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA \$0.00 **FY01 BA** \$0.00 **FY02 BA** \$219,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0202030

FWP and possible subtask under FWP:
Integrated Modeling of Novel Materials

FWP Number: 04SCPE420

Program Scope:
The design of novel electronic and structural materials to satisfy current and future civilian and military technology needs requires multi-technique and interdisciplinary approaches that qualitatively extend the existing theory and modeling base; our emphasis is on using and controlling intrinsic multiscale complexity in strongly correlated electronic materials. We emphasize development and application of advanced techniques drawn from combinations of many-body, local density, molecular dynamics and other techniques, capable of predictive descriptions of tunable classes of complex electronic materials. The techniques are applied in a closed-loop of formulating and solving minimal models, and testing predictions against experimental data (including use of major DOE facilities, especially pulsed neutrons, high magnetic fields, and high-performance computing), with the aim of identifying, understanding, and controlling the underlying synthesis-microstructure-property relations.

Major Program Achievements (over duration of support):
Developed and applied cutting-edge analytical and numerical methods for many-body models appropriate to collective broken-symmetry ground states and excitations in new classes of strongly correlated materials, including conjugated organics, charge-transfer complexes, transition metal oxides (high-Tc superconductors, colossal magnetoresistance manganites, ferroelectrics, etc.), actinides, martensites, and nanoscale materials.

Program Impact:
Applied advanced modeling and simulation tools to interpret and guide modern experimental probes of multiple spatial and temporal scales, including time-of-flight neutrons, high-intensity light sources, high magnetic fields, ultrafast time-resolved optical and vibrational spectroscopies, and scanning-tunneling microscopies. 102 publications and 59 invited talks in past two years.

Interactions:
Several single- and multi-campus funded collaborations with U. California and other major Universities. Extensive visitor, student, and postdoctoral program. Internal (LANL) collaborations include those with LANSCE, NHMFL, MST and T divisions. External collaborators include E. Abrahams (Rutgers), D. Scalapino (UC Santa Barbara), J. R. Schrieffer (Florida State), S. Davis (UC Berkeley), R. Laughlin and Z. X. Shen (Stanford), S. Chakravarty (UCLA), P. Bourges (Saclay), J. Zaanen (Leiden), M. Roukes (Caltech), J. Wilkins (Ohio State), J. A. Krumhansl (Cornell University), and L . Sham (UC San Diego).

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
A. Bishop, E. O. Lawrence Award in Materials Science (1993)
G. Ortiz, Fellow of the Institute of Physics, England (2001)
S. Trugman, LANL Fellows Prize, outstanding research (1996)

Personnel Commitments for FY2002 to Nearest +/- 10%: R.C. Albers (10%), A.V. Balatsky (20%), A.R. Bishop (10%), J.E. Gubernatis (20%), I. Martin (10%), G. Ortiz (10%), S.A. Trugman (20%).

Authorized Budget (BA) for FY00, FY01, FY2002:
FY00 BA $354,000 FY01 BA $287,000 FY02 $178,700

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0202030

FWP and possible subtask under FWP:
Accelerated Atomistic Simulation of Defect Dynamics

FWP Number: 04SCPE420

Program Scope:
A long-standing and crucial problem in the atomistic simulation of materials is the limited time scale available to these simulations. While molecular dynamics can reach nanoseconds, important activated processes in realistic systems often occur on time scales of microseconds, milliseconds, and longer. Examples include diffusion and reorganization events during film growth, annealing of the highly strained defect region after a radiation damage event, and defect mobility in carbon nanotubes. Building on sound statistical mechanics principles, we are developing new approaches for extending this simulation time. These "accelerated molecular dynamics" methods (hyperdynamics, parallel replica dynamics, and temperature accelerated dynamics) offer a way to reach experimentally relevant time scales without any prior knowledge of what activated events might occur. We are developing these methods into a powerful tool set for studying real materials problems and collaborating with experts to apply them in a number of fields.

Major Program Achievements (over duration of support):

- Developed the parallel replica method, which harnesses the power of parallel processing to reach longer simulation times for infrequent-event systems (contrary to the sequential-time paradigm).
- Developed the temperature accelerated dynamics (TAD) method, which can reach boost factors thousands and millions over regular molecular dynamics when relative activation barriers are high.
- Applied TAD to the first realistic simulations of vapor-deposited crystal growth, matching the experimental temperatures and deposition rates (slower than monolayers per second) with no prior assumptions about mechanisms.
- Showed that parallel-replica dynamics can be applied to driven systems.
- Discovered the perpendicular steering effect, in which a surface roughening instability results from deposition at very low incoming velocity, and a shuffle effect.

Program impact:
With these new methods, we are getting the first glimpses of processes on time scales that were heretofore inaccessible. For virtually every system we have examined so far, unexpected behavior was discovered. We are now beginning to see this effect in a broader range of fields as we put the methods into the hands of experts outside Los Alamos. We regularly receive invitations to talk at universities and national and international conferences, write book chapters, etc., and to collaborate on proposals to national funding agencies. These methods are beginning to show up in textbooks. We have a CRADA with Motorola corporation to apply these methods to understand and develop next-generation electronic devices. Also: organized symposium on extended-scale simulation methods at the 2002 International Conference on Computational Nanoscience.

Interactions:
Steve Stuart (Clemson), Jim Sprague (NRL), Francesco Montalenti (Milano), Yuri Mishin (George Mason), John Hamilton (Sandia), Kai Nordlund (Helsinki), David Sholl (Carnegie Mellon), Walter Rudd (Oregon State), Wolfgang Windl (Ohio State), Jim Adams (ArizonaState), John Wilkins (Ohio State), Hannes Jonsson (Washington/Iceland), Richard Hoagland (Washington State, now LANL), Riccardo Ferrando (Genova), Jacques Amar (Toledo), Intel Corporation, Motorola Corporation.

Recognitions, Honors and Awards :
A.F. Voter: Editorial board of Theoretical Chemistry Accounts (2001-2002, 2003-2004).

Personnel Commitments for FY2002 to Nearest +/- 10%:
A.F. Voter (PI) 90%, B.P. Uberuaga (postdoc) 100% (paid by Motorola CRADA), G. Henkelman (postdoc) 20% (unpaid by DOE), M. Anghel (postdoc) 40% (unpaid by DOE), T.C. Germann (staff member) 10% (unpaid by DOE), S. Swaminarayan (staff member) 10%.

Authorized Budget (BA) for FY00, FY01, FY02:

FY00 BA $280,000	FY01 BA $302,000	FY02 $327,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0201030

FWP and possible subtask under FWP:
Metastable Phases and Microsctructures

FWP Number: 04SCPE419

Program Scope:
The program focuses on attaining an atomic-level understanding and predictive capabilities for materials with metastable microstructures and bulk metallic glasses, which have the potential to make significant contributions to energy-efficient technologies. The program studies the synthesis of bulk metallic glasses, studying homogeneous and heterogeneous nucleation of crystals in undercooled metallic melts. The use of fluxes to remove heteronucleants is being investigated. The mechanical properties of the bulk glasses are studied with the purpose of deriving a microscopic understanding of plasticity in amorphous materials. For this, macroscopic stress-strain observations are complemented by microscopic studies using atom probe field-ion microscopy and molecular-dynamics computer simulation. The research also addresses the properties of metal and ceramic powders with fine microstructures. Mechanical alloying (a high-energy ball milling technique) is used to prepare metal and ceramic powders, which are investigated as such or after consolidation by hot pressing and/or HIPping.

Major Program Achievements (over duration of support):
Bulk metallic glasses: Perfected a fluxing method for the synthesis of bulk metallic glasses. Used X-ray photoelectron spectroscopy to study the electronic structure in Pd-based metallic glasses; Studied the effect of plasticity on the elastic modulus and density of bulk amorphous alloys; Used molecular dynamics with a modified embedded-atom potential to study solidification and crystallization in undercooled melts; Used atom-probe tomography to study the early decomposition of a bulk metallic glass.
Thin films: Used Rayleigh waves to study the anomalous elastic properties at metal-metal interfaces as it relates to the supermodulus effect and the elastic properties of nanostructured materials.
Hydrogen Storage: Developed a thermodynamic model to explain the ubiquitous hysteresis in the absorption/desorption of hydrogen in metals; Developed Mg-based alloys for hydrogen storage.
Metastable Materials: Studied the synthesis and properties of Vanadium-Spinel composites for structural applications in high radiation environments.

Program Impact: The present program was seminal for obtaining new funding from DOE's Carbon Initiative program for research on "Bulk Ferromagnetic Glasses". Schwarz co-organized the 12th International Conf. on the Strength of Metals and Alloys, Asilomar, CA, August 2000. Schwarz co-organized a MRS symposium on "Materials for Energy Storage, Generation, and Transport", February 2002.

Interactions: Profs. T. Tiainen, V.T. Kuokkala, P. Ruuskanen, and J. Vuorinen (Tampere Univ. of Technology, Finalnd); Prof. W. Nix (Stanford Univ.); Prof. A. Khachaturyan (Rutgers Univ.); Profs. R. Ritchie and V. Schroeder (UC-Berkeley), Prof. T. Egami (Univ. Penn); Prof. A Granato (Univ. Ill., Urbana); Profs. David Williams and H. Jain (Lehigh Univ.); Prof. J. Williams and V. Sinha (Ohio State Univ.); Dr. M. K. Miller (ORNL); *Internal LANL:* - M. Hundley, J. Thompson, D. Taylor, M. Baskes, M. Nastasi, Y. Zhao, F. Cherne.

Recognitions, Honors and Awards: (at least partly attributable to support under this FWP or subtask):
In 1995, R. B. Schwarz was elected *Fellow* of the American Society for Metals (ASM). In 2002, R. B. Schwarz was elected *Fellow* of The Mineral, Metals and Materials Society (TMS). In 2002, R. B. Schwarz was awarded a "Honorary Doctor of Technology" degree by the Tampere University of Technology, Finland.

Personnel Commitments for FY2002 to Nearest +/- 10%:
R. B. Schwarz (25%), T. D. Shen (60%)

Authorized Budget (BA) for FY00, FY01, FY2002:
FY00 BA $323,000 **FY01 BA** $290,000 **FY02 BA** $285,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0201030

FWP and possible subtask under FWP:
Ferromagnetic Alloys

FWP Number: 04SCPE478

Program Scope:
We study bulk ferromagnetic amorphous alloys with potential use in energy conversion devices such as electrical transformers and motors. Currently, about 1% of the total electrical energy produced in the U.S. is lost as heat dissipated by distribution transformers, motors, and other electrical energy conversion devices. These losses can be substantially decreased by the use of more efficient transformers and motors that use ferromagnetic cores made from amorphous (glassy) materials. Existing amorphous foils prepared by rapid quenching techniques are at most 40 μm thick. However, the optimum implementation of ferromagnetic glasses requires that these materials be prepared in the form of laminas at least 0.3-mm thick. Then program focuses on obtaining a fundamental understanding of the synthesis and properties of bulk ferromagnetic alloys. We study homogeneous and heterogeneous nucleation of crystals in undercooled metallic melts; the use of fluxes to remove heteronucleants; and the magnetic properties (coercivity, magnetic moment, cyclic hysteresis losses) of the ferromagnetic alloys prepared under this program.

Major Program Achievements (over duration of support):
Developed a magnetic phase diagram for amorphous Pd(40)-Ni(40)-Fe(x)-P(20) (x=0-17.5) alloys. We found that with decreasing temperature, these alloys become paramagnetic, superparamagnetic and spin glasses. At low temperatures there is also an induced ferromagnetic state [J. Appl. Phys. 85(1999)4110]. Using a flux melting technique we prepared bulk ferromagnetic alloys containing between 62 and 71 at.% Fe [Appl. Phys. Letters 75(1999)49]. We demonstrated that the ferromagnetic glass Fe(40)-Ni(40)-P(14)-B(6), previously studied as thin ribbon, can be made in bulk form provided one removes heteronucleants by fluxing. All properties of the bulk glass are similar to those of the thin foils except the rate of crystal nucleation, which is four orders of magnitude lower in the bulk glass than in the rapidly quenched ribbons [Acta mater. 49(2001)837]. The large magnetic entropy of ferromagnetic glasses makes them suitable for applications in magnetic refrigeration. We studied the magnetocaloric effect in Pd-Ni-Fe-P amorphous alloys as a function of temperature and magnetic field. The entropy change at 80K and 50 kOe is comparable to that found in other crystalline and amorphous Fe-based alloys [J. Appl. Phys. 91(2002)5240].

Program Impact: Schwarz co-organized the 12th International Conf. on the Strength of Metals and Alloys, Asilomar, CA, August 2000. Schwarz co-organized a MRS symposium on "Materials for Energy Storage, Generation, and Transport", February 2002. On the average, we have been asked to present three invited talks per year at national and international conferences.

Interactions: Profs. T. Tiainen, V.T. Kuokkala, P. Ruuskanen, and J. Vuorinen (Tampere Univ. of Technology, Finalnd); Prof. W. Nix (Stanford Univ.); Prof. A. Khachaturyan (Rutgers Univ.); Profs. R. Ritchie and V. Schroeder (UC-Berkeley), Prof. T. Egami (Univ. Penn); Prof. A Granato (Univ. Ill., Urbana); Profs. David Williams and H. Jain (Lehigh Univ.); Prof. J. Williams and V. Sinha (Ohio State Univ.); Dr. M. K. Miller (ORNL); *Internal LANL:* - M. Hundley, J. Thompson, D. Taylor, M. Baskes, M. Nastasi, Y. Zhao, F. Cherne.

Recognitions, Honors and Awards: (at least partly attributable to support under this FWP or subtask):
In 1995, R. B. Schwarz was elected *Fellow* of the American Society for Metals (ASM). In 2002, R. B. Schwarz was elected *Fellow* of The Mineral, Metals and Materials Society (TMS). In 2002, R. B. Schwarz was awarded a "Honorary Doctor of Technology" degree by the Tampere University of Technology, Finland.

Personnel Commitments for FY2002 to Nearest +/- 10%:
R. B. Schwarz (50%), T. D. Shen (20%), U. Harms (100%), J. I. Archuleta (40%)

Authorized Budget (BA) for FY00, FY01, FY2002:

FY00 BA $426,000	FY01 BA $388,000	FY02 BA $380,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0202020

FWP and possible subtask under FWP:
Microscopic Characterization of Buried Interfaces using Magnetic Resonance Force Microscopy

FWP Number: 04SCPE451

Program Scope: The magnetic resonance force microscope (MRFM) is a novel scanned probe instrument that combines the three-dimensional imaging capabilities of magnetic resonance imaging with the high sensitivity and resolution of atomic force microscopy. It will enable non-destructive, chemical-specific, high-resolution microscopic studies and imaging of subsurface properties of a broad range of materials. Our unique cryogenic fully scanning MRFM will soon incorporate sophisticated high frequency, surface nanomachined microresonators with integral sub-micron probe magnets. The use of electronic spin promises new capabilities for information processing based on new magnetic materials and devices with unprecedented capabilities and levels of performance that are being created by tailoring the structure and composition of multi-component materials at the nanometer scale. The buried interfaces between the various components of these new materials play a central role in determining their functional behavior. We are applying the MRFM to problem of spin-based electronics with the goal of better gaining an improved understanding of their buried interfaces and microstructure, and exploring the potential of a single spin MRFM for characterization and readout of spin-based quantum computer.

Major Program Achievements (over duration of support):
First demonstration of MRFM detection of Ferromagnetic Resonance ["Observation of Ferromagnetic Resonance in a Microscopic Sample Using Magnetic Resonance Force Microscopy," *Appl. Phys. Lett.* 68, 2005 (1996)].
Implementation of only low temperature, fully scanning magnetic resonance microscope
Demonstration of 1000 electronic moment spin sensitivity ["Magnetic Resonance Force Microscopy and the Solid State Quantum Computer," *SPIE Proceedings, Optical Engineering*]
Development of a novel micromagnetic probe tip fabrication process (submitted for patent).
First microscopic study of thin Co films ["Ferromagnetic Resonance Force Microscopy on Microscopic Co Single Layer Films," *Appl. Phys. Lett.* 73, 2036 (1998)].
Demonstration of MRFM detected Co NMR
Discovery and analysis of MRFM/ferromagnetic resonance imaging in ferromagnet
Establishment of spin-based solid state quantum computer collaboration based on MRFM single spin readout and characterization; formed basis for successful FY00 LDRD DR proposal.
First quantitative analysis of interactions between magnetic probe and bulk samples in magnetic resonance force microscopy ["Probe-Sample Coupling in the Magnetic Resonance Force Microscope," *Journal of Magnetic Resonance* 154, 210 (2002)].
Studies of MRFM-based quantum computing ["Magnetic resonance force microscopy quantum computer with tellurium," *Phys. Rev. Lett.* 86, 2894 (2001)].

Program Impact: Chris Hammel was recently named Ohio Eminent Scholar and Professor of Physics at Ohio State University, was appointed LANL Fellow, was awarded the LANL Fellows Prize, is a member of the Quantum Information Science and Technology Experts Panel, was elected to the executive committee of the Instrumentation and Measurement Science Topical Group of the American Physical Society, and is a Visiting Associate at Caltech. Hammel has presented 31 invited talks on MRFM: 3 APS March meeting and 2 Gordon Conference invited talks, 12 invited talks at international workshops and conferences, and 14 invited talks at Universities throughout the world.

Interactions: Michael Roukes (Caltech); Bob Clark (UNSW), Keith Schwab and Bruce Kane (Lab for Physical Studies, Maryland) and Richard Hughes (LANL) (solid state quantum computer); Ivar Martin and Gennady Berman (LANL); Philip Wigen, (Ohio State Univ.), Bret Heinrich (Simon Fraser University), Michael Fitzsimmons [LANL, E355]

Personnel Commitments for FY2002 to Nearest +/-10%:
P.C. Hammel, staff, 25%; D. Pelekhov, staff, 50%; Y. Obukhov, Postdoc, 100%; visitor Phil Wigen (Ohio State Univ. 10%); 2 students at Caltech, 100%; and 1 postdoc at Caltech, 100%

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $641,000 **FY01 BA** $648,000 **FY02 BA** $503,000

Laboratory Name: Los Alamos National Laboratory
B&R Code: KC0201020

FWP and possible subtask under FWP:
Deformation Physics of Ultrafine Scale Materials

FWP Number: 04SCWE486

Program Scope: This program investigates the new deformation physics of ultrafine scale materials with strengths near the theoretical limits via a highly synergistic combination of atomistic simulations and experimental methods. Initial focus is on nanolayered metallic composites and the integrated approach consists of synthesis by vapor deposition; structure-property correlations by means of transmission electron microscopy, x-ray diffraction, microtensile and nanoindentation testing; and atomistic simulations of dislocation behavior involved in the deformation at nanoscales.

Major Program Achievements (program started in FY00, with full funding in FY01)**:**
Nanoscale design of metals with strengths approaching the theoretical limit: An increase of up to two orders of magnitude in strength over bulk materials is observed when the structural scale of the nanolayer composites is reduced to a couple nanometers. Atomistic simulations reveal that new deformation mechanisms involving complex interactions of single dislocations (as opposed to pile-up) with the strain fields at coherent or semi-coherent interfaces give rise to such high strengths.
New deformation textures were discovered in nanolayered Cu-Nb composites cold rolled to high plastic strains consistent with a coordinated single slip mechanism, in which the interface plays a critical role in the homogeneous distribution of slip.
Thermal stability: Cu/Nb nanolayers reveal unusual morphological stability of the layer structure to homologous temperatures as high as 80% of the absolute melting point of Cu via a new mechanism of synchronized grooving and shear at triple points that “anchor” the grain boundaries.

Program impact: This program has already led to discoveries of new regimes of plasticity in nanoscale composite materials that will require new scientific models to understand the mechanical behavior of nanoscale materials exhibiting strengths near the theoretical limit. The work from this program is largely the basis for the nanomechanics thrust area in the upcoming Center for Integrated NanoTechnologies in New Mexico. The scientific knowledge from this program should impact a broad range of engineering materials, from load-bearing structural components to micro and nano electro-mechanical systems.

Interactions:
P.M. Anderson (Ohio State University), A.K. Mukherjee (UC, Davis), T. Ungar (Eotvos University Budapest, Hungary), T. Foecke (NIST), G. Pharr (ORNL/U-Tennessee), Julia Weertman (Northwestern University), H. van Swygenhoven (Paul Scherrer Institute, Switzerland), P. Peralta (Arizona State University), Charles Barbour, D. Follestaedt (SNL, Albuquerque).

Recognitions, Honors and Awards (since FY’00):
R.G. Hoagland, PNNL, Matthias scholar at LANL, FY’00
P.M. Anderson, Ohio State University, Matthias scholar at LANL, FY’02.
F. Spaepen, 1999 Humboldt Research Award for Senior U.S. Scientists,
F. Spaepen, 2002 Robert Franklin Mehl Award, The Minerals, Metals & Materials Society (TMS)
24 refereed publications, 1 plenary presentation, 10 invited talks at national/ international symposia, 4 symposia/workshops organized (MRS Fall 2000, United Engineering Foundation, Italy, 2001, TMS Annual 2003, MRS Spring 2003), edited MRS Bulletin issue on *Mechanical Properties of Nanostructured Materials*, 1999.

Personnel Commitments for FY2002 to Nearest +/- 10%:
H. Kung (change-of-station to DOE), A. Misra (LANL, 50%), R.G. Hoagland (LANL/PNL, 35%), J.D. Embury (McMaster University, 10%), J. P. Hirth (LANL-Affiliate, 10%), T. Yamamoto (LANL, postdoc, 100% till 03/2002), X. Zhang (100%, since 04/2002, LANL Director’s funded post-doc fellow), Prof. F. Spaepen, (Harvard University, 5%), Denis Yu (100%, GRA, Harvard University), R.J. Kurtz (PNNL, 25%), and C.H. Henager, Jr. (PNNL, 25%)

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA \$266K **FY01 BA** \$591K LANL+ \$138K PNNL **FY02 BA** \$469K LANL+ \$131K PNNL